

Supporting Information

Dendritic Anion Hosts: Perchlorate Uptake by G5-NH₂ Poly(propyleneimine) Dendrimer in Water and Model Electrolyte Solutions.

Environmental Science and Technology

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Table S1. Selected Properties of Perchlorate and Related Anions.

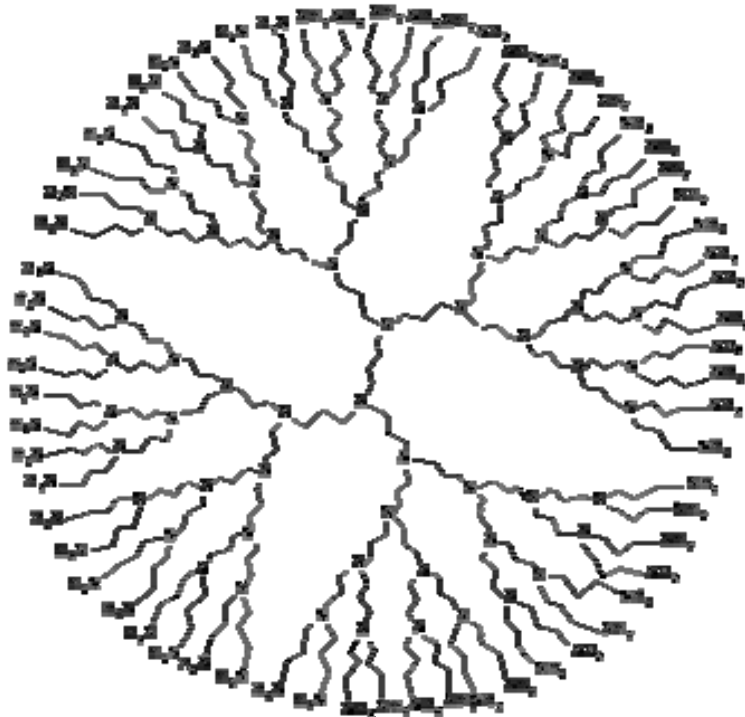
Anion	^a Ionic Radius (nm)	^b Charge-to-Size Ratio	^a Hydration Free Energy (kJ/mol)	^c Shape
ClO ₄ ⁻	0.240	-4.17	-205	Tetrahedral
Cl ⁻	0.172	-5.81	-340	Spherical
NO ₃ ⁻	0.196	-5.10	-300	Trigonal Planar
HCO ₃ ⁻	0.156	-6.41	-335	Trigonal Planar
SO ₄ ²⁻	0.230	-8.69	-1295	Tetrahedral

^aData compiled by Moyer, B. A. and Bonnese, P. V. Physical factors in anion separations. In *Supramolecular Chemistry of Anions*. Bianchi, A.; Bowman-James, K. and Garcia-Espana, E. Ed.; Wiley-VCH, New York, 1997, pp 1-44.

^bEqual to the ratio of the charge of the anion to its ionic radius.

^cGeometrical arrangements of anions taken from Gloe, K.; Stephan, H. and Grotjahn, M. Where is the anion extraction going? *Chem. Eng. Technol.* **2003**, 26,1107-1117.

Figure S1: 2-D Structures of PPI and PAMAM dendrimers.
A. G5-NH₂ PPI Dendrimer



B. G4-NH₂ PAMAM Dendrimer

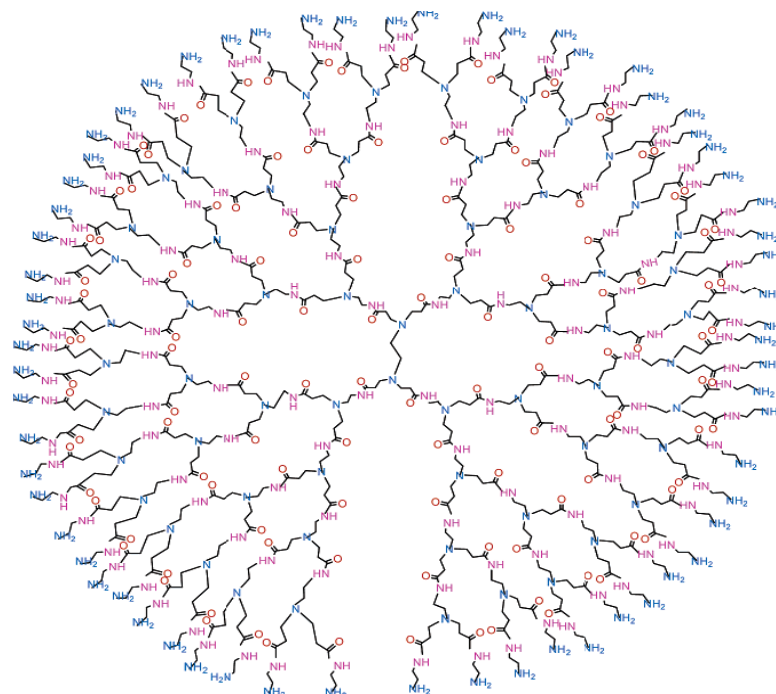


Figure S2: Fractional binding of perchlorate to G5-NH₂ PPI and G4-NH₂ PAMAM dendrimers in deionized water. The initial perchlorate concentration in solution is 1000 ppb (0.01 mM).

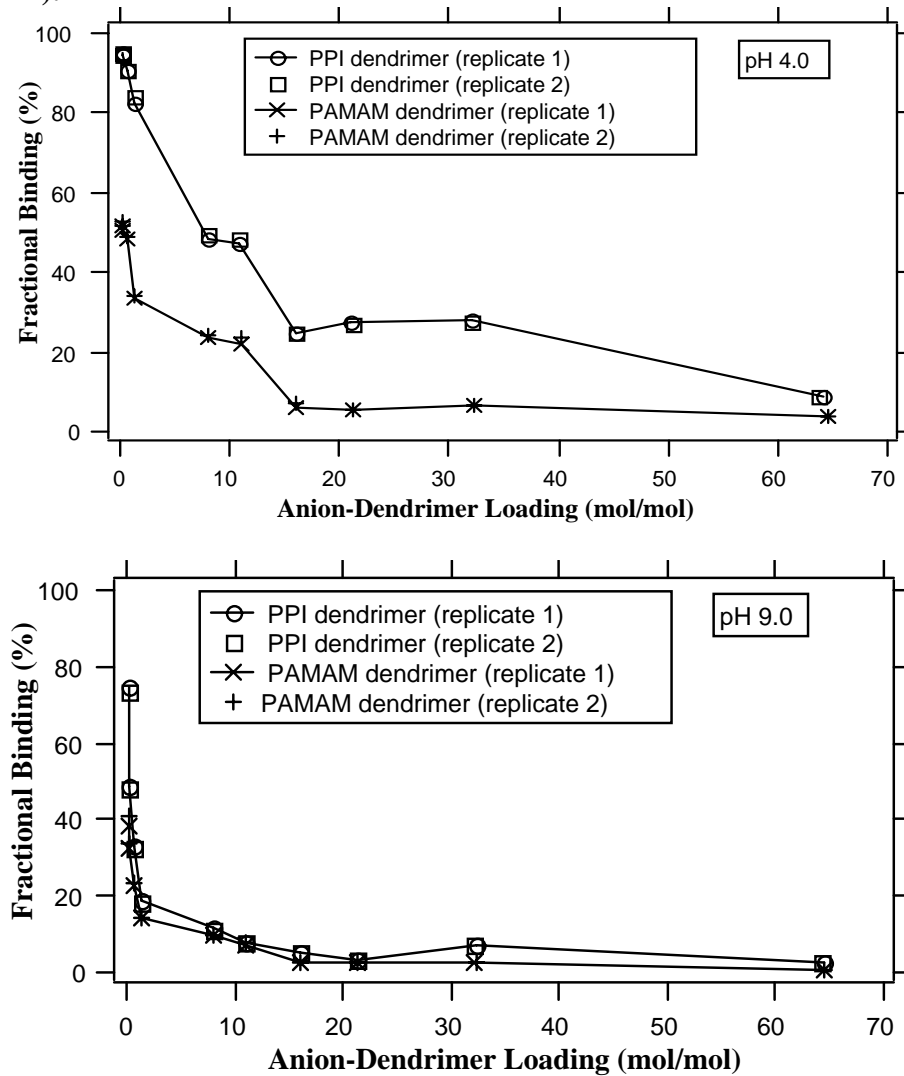


Figure S3: Fractional binding of perchlorate to G5-NH₂ PPI dendrimer in deionized water and model electrolyte solutions at room temperature and reaction time of 1 hr. The initial perchloration concentration in solution is 1000 ppb (0.01 mM). Electrolyte 1 consists of an aqueous solution containing 0.1 mM NaCl, 0.3 mM NaHCO₃, 0.1 mM NaNO₃ and 0.1 mM Na₂SO₄. Electrolyte 2 consists of an aqueous solution containing 1.0 mM NaCl, 3.0 mM NaHCO₃, 1.0 mM NaNO₃ and 1.0 mM Na₂SO₄.

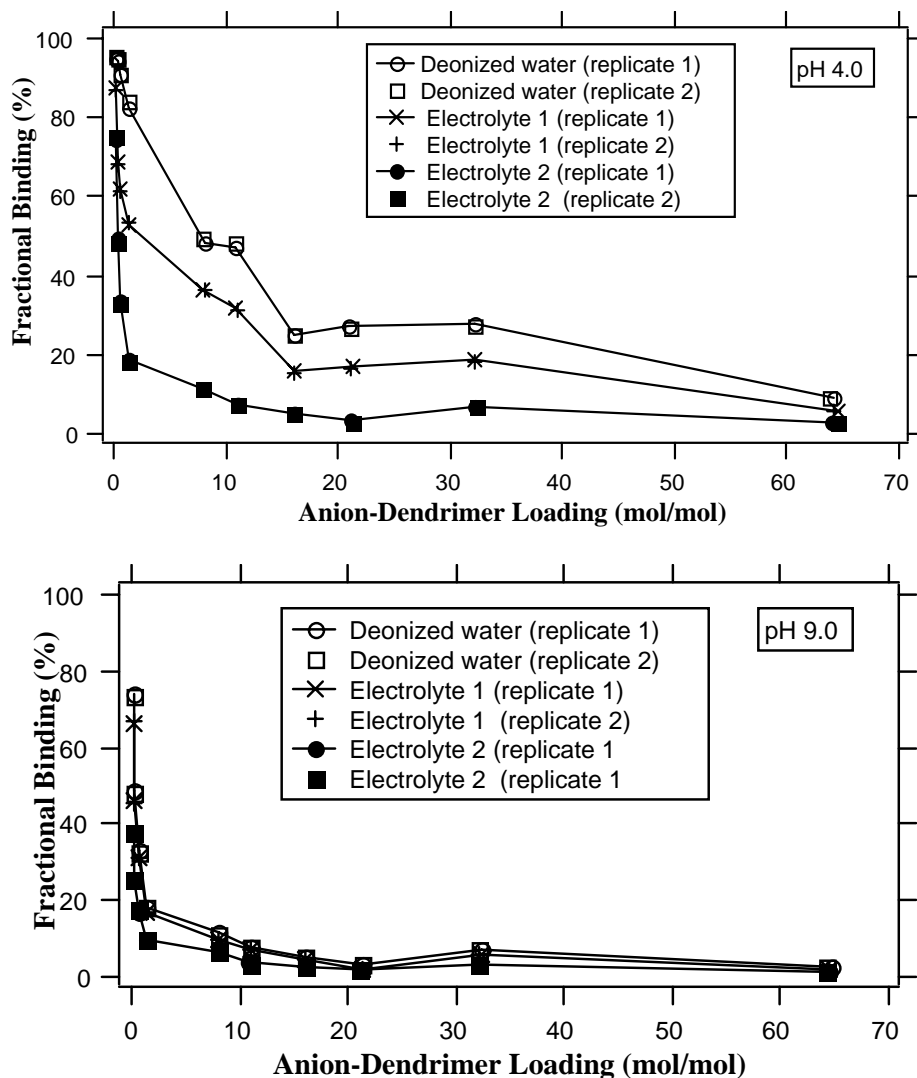


Figure S4: Fractional binding of perchlorate to G5-NH₂ PPI dendrimer in deionized water, electrolyte and mixture of electrolyte + G4-NH₂ PAMAM dendrimer at room temperature and reaction time of 1 hr. The initial perchloration concentration in solution is 1000 ppb (0.01 mM). The electrolyte consists of an aqueous solution containing 1.0 mM NaCl, 3.0 mM NaHCO₃, 1.0 mM NaNO₃ and 1.0 mM Na₂SO₄.

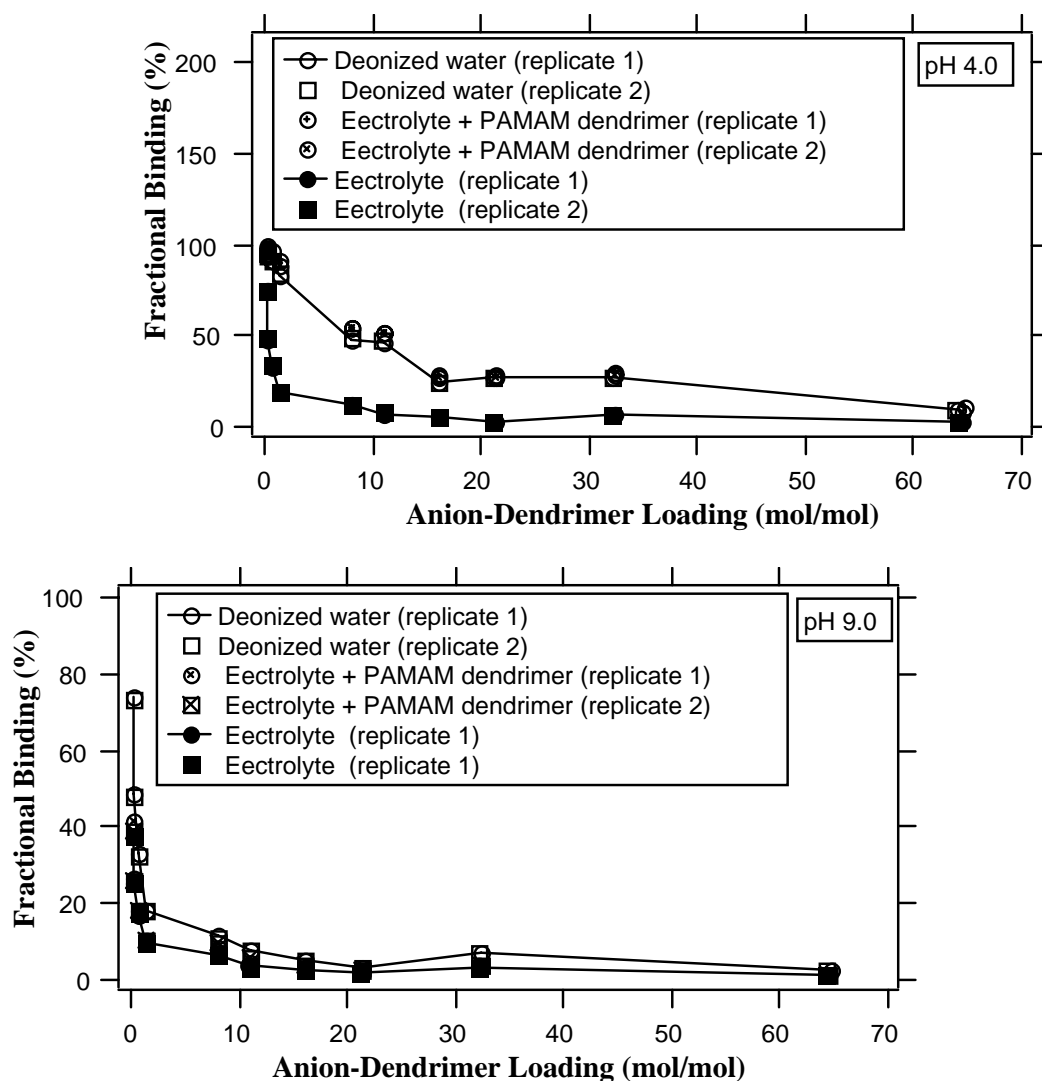


Figure S5: Fractional binding of perchlorate to G5-NH₂ PPI dendrimer in deionized water and electrolyte at room temperature as a function of reaction time. The initial perchloration concentration in solution is 1000 ppb (0.01 mM). The electrolyte consists of an aqueous solution containing 1.0 mM NaCl, 3.0 mM NaHCO₃, 1.0 mM NaNO₃ and 1.0 mM Na₂SO₄.

